Stochastic Equations and Processes in physics and biology

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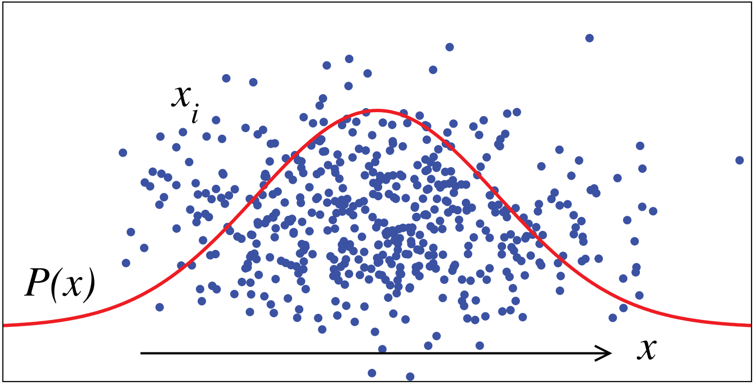
Examples of stochastic networks

- Social networks
- Transport networks
- Groups of animals or humans
- Colonies of living microorganisms
- Interacting particles: in gasses and liquids
- Magnetism
- Neural networks: e.g. epileptic seizure, AI.

Global effects

Global effects in coupled networks



Global effects

Global effects in coupled networks

- Phase transitions (e.g. gas to liquid)
- Clustering (spatial phase separation)
- Synchronization (oscillations)

Global effects

Coordinates of individual elements

$$x_i, \qquad (i = 1, \ldots, N)$$

Number density function

$$\rho(x,t) = \frac{\text{number of elements}}{\text{volume}}$$

Mean field as a measure of global state

$$\langle x \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i = \int_V x \rho(x,t)\, dx$$

Dynamic stochastic network

Coupling matrix C_{ik} in a 1D network

$$\dot{x}_i = -\frac{dU(x_i)}{dx_i} + \sum_{k=1}^{N} C_{ik} f(x_k^\tau) + \sqrt{2D}\xi_i(t)$$

Mean-field coupling

$$\dot{x}_i = -\frac{dU(x_i)}{dx_i} + \frac{h(x_i)}{N} \sum_{k=1}^{N} f(x_k^\tau) + \sqrt{2D}\xi_i(t)$$

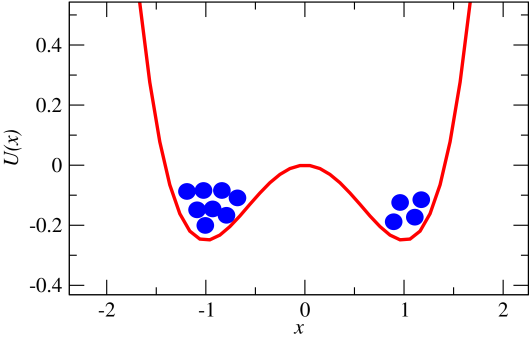
Global pair-interaction

$$\dot{x}_i = -\frac{dU(x_i)}{dx_i} - \sum_{k=1}^{N} \frac{\partial W(\|x_i - x_k\|)}{\partial x_i} + \sqrt{2D}\xi_i(t)$$

System of globally coupled bistable elements

Double-well potential

$$U(x) = \frac{x^4}{4} - \frac{x^2}{2}$$

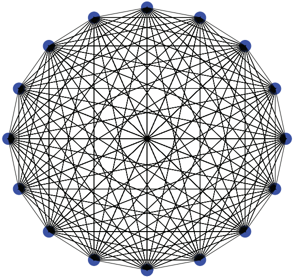


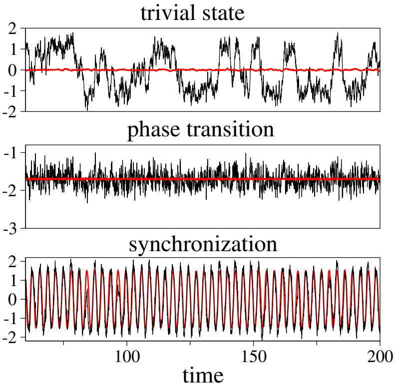
Linear mean-field coupling

$$\dot{x}_i = -\frac{dU(x_i)}{dx_i} + \alpha\frac{1}{N}\sum_{k=1}^{N} x_k + \sqrt{2D}\xi_i(t)$$

System of globally coupled bistable elements

All-to-all coupling: phase transitions and synchronization





System of globally coupled bistable elements

Molecular chaos approximation

$$P_N(x_1, x_2, x_3, ..., x_N, t) = P(x_1, t)P(x_2, t)...P(x_N, t)$$

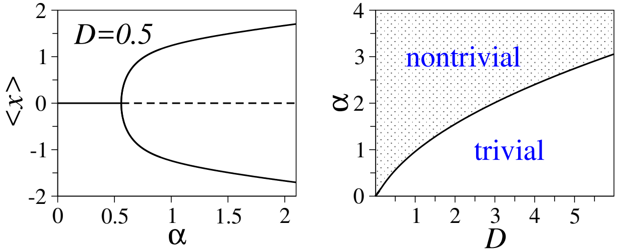
One particle distribution function

$$P(x, t) = \int_G P_N(x_1, x_2, x_3, ..., x_N, t)\, dx_1\, dx_2 \ldots dx_{N-1}$$

Nonlinear Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial x}\left[\frac{dU}{dx}P - \alpha\langle x\rangle P + D\frac{\partial P}{\partial x}\right], \quad \langle x\rangle = \int_G xP(x, t)\, dx$$

Phase transitions in symmetric bistable potential



Second-order phase transition occurs at $D = \alpha \int P_s(x) x^2 \, dx = \alpha \langle x^2 \rangle_0$

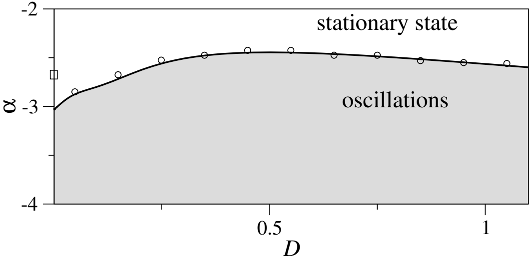
$$P_s(x) = C \exp\left(\frac{-U(x) + \alpha\langle x\rangle}{D}\right), \quad \langle x\rangle = \int_{-\infty}^{\infty} x P_s(x)\, dx$$

Synchronization in a network of bistable elements with time delay mean field coupling

Mean-field coupling with time delay

$$\dot{x}_i = -\frac{dU(x_i)}{dx_i} + \alpha \frac{1}{N} \sum_{k=1}^{N} x_k(t-\tau) + \sqrt{2D}\xi_i(t)$$

Synchronization threshold



[A. Pototsky and N. Janson, Physica D: Nonlinear Phenomena, **238**, 175–183 (2008)]

Enhanced rectification of attracting particles in a single-file

- A. Pototsky, A. J. Archer, M. Bestehorn, D. Merkt, S. Savel'ev, and F. Marchesoni Phys. Rev. E 82, 030401(R), (2010)
- Andrey Pototsky, Andrew J. Archer, Sergey E. Savel'ev, Uwe Thiele, and Fabio Marchesoni Phys. Rev. E 83, 061401 (2011)

Diffusion under structural confinement

Standard $1d$ diffusion of a single Brownian particle

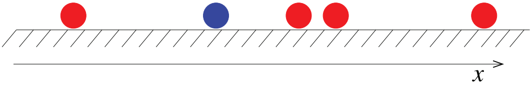
$$\lim_{t\to\infty}\langle (x-x_0)^2\rangle = 2Dt,$$

$D\ldots$ **diffusion coefficient**

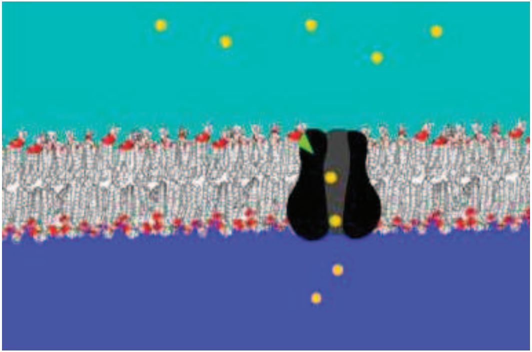
Diffusion in a single file: no passing through the particles

$$\lim_{t\to\infty}\langle (x-x_0)^2\rangle = 2F\sqrt{t},$$

$F\ldots$ **mobility of a single file**

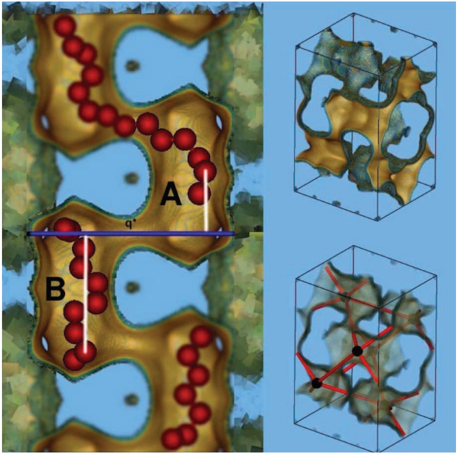


Calcium channel in a cell membrane



Voltage-gated channel for Ca^{2+} found in excitable cells (muscles, neurons)

Porous materials: zeolites



Schematic diagram of the diffusion of linear alkanes in Erionite (ERI), [D. Dubbledam *et al.*, PRL 90 245901 (2003)]

Artificial single-file motion

Highly-diluted aqueous solution of sulphate-terminated polystyrene particles with $2.9\ \mu$m diameter.

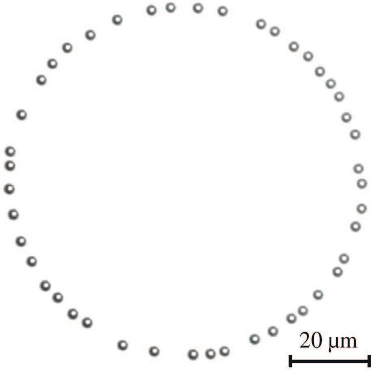
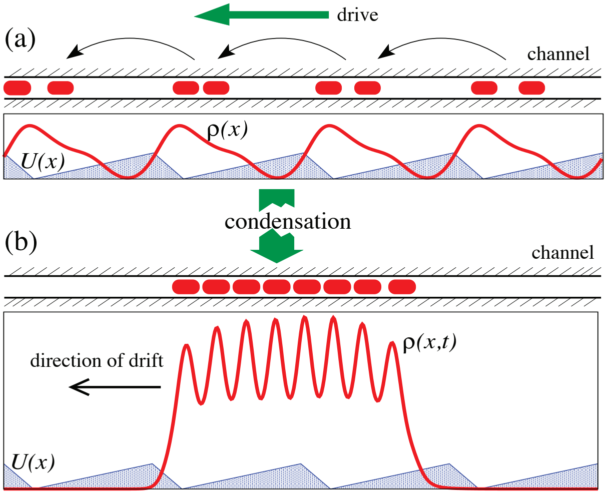


Image of colloidal particles trapped by a scanning laser beam to a circular optical trap,

[C. Lutz *et al.*, PRL 93 026001 (2004)]

Brownian motion in a single file



$U(x)\ldots$ Channel potential,

$\rho(x,t)\ldots$ distribution density of the number of particles

Brownian motion in a single file

Langevin equations

$$\dot{x}_i \quad = \quad -\frac{dU(x_i)}{dx_i} + A(t) - \frac{\partial \Phi(\{x_j\})}{\partial x_i} + \sqrt{2T}\xi_i(t), \;\; i = 1 \ldots N$$

Stochastic term and interaction energy

$$\langle \xi_i(t)\xi_i(t')\rangle = \delta(t-t'), \quad \Phi(\{x_j\}) = \frac{1}{2}\sum_{j\neq i}\sum_{i} w(\mid x_i - x_j \mid)$$

Pair interaction potential

$$w(x_{ij}) = w_{\mathrm{hr}}(x_{ij}) + w_{\mathrm{at}}(x_{ij}), \quad x_{ij} = \mid x_i - x_j \mid$$

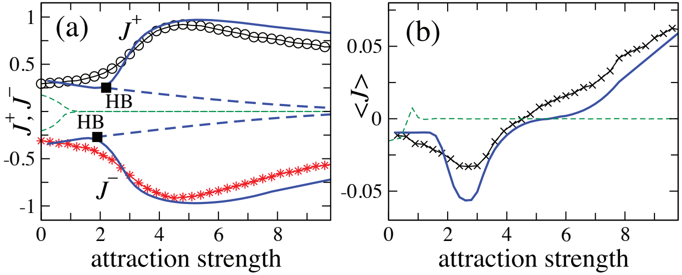
Ratchet potential and boundary conditions

$$U(x) = \sin{(2\pi x)} + \frac{1}{4}\sin{(4\pi x)}, \quad \text{system size} \ldots S = M, \;\; w(S) \approx 0.$$

Constant drive $A(t) = A = const$: unidirectional currents

$$\frac{\partial \rho(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}, \quad J^{\pm} = \frac{1}{Nt} \lim_{(t\to\infty)} \int_{t'}^{t'+t} dt \int_{-S/2}^{S/2} J^{\pm}(x,t)\, dx$$

DDFT *vs* BD simulation



Brownian motion in a single file

1. Symmetry breaking

spontaneous increase of the attraction strength

2. Depinning

(a) weak attraction (close to the Hopf point)

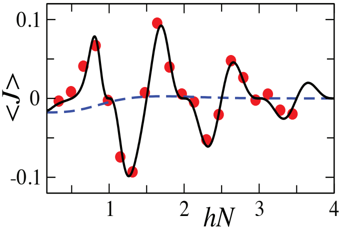
(b) strong attraction

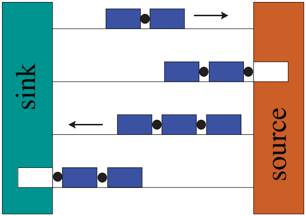
Brownian motion in a single file

Strong attraction limit

$$\frac{dy}{dt} = -\frac{U(y+hN) - U(y)}{hN} + A(t) + \sqrt{\frac{2T}{N}}\xi(t), \quad y = \frac{1}{N}\sum_i x_i$$

Efficiency of the low-frequency transport

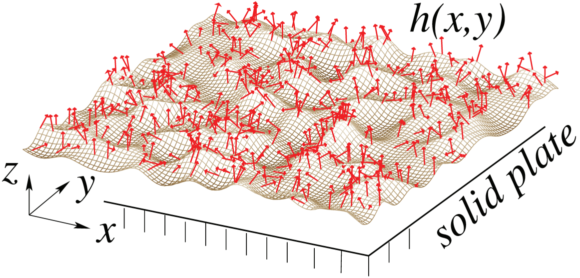




Models of biofilms

- *Swarming of self-propelled particles on the surface of a thin liquid film*, A. Pototsky, U. Thiele and H. Stark, Edited by: E. Scholl, E, SHL. Klapp, P. Hovel, CONTROL OF SELF-ORGANIZING NONLINEAR SYSTEMS Book Series: Understanding Complex Systems Springer Complexity, Pages: 393-412, Springer-Verlag (2016)
- *Mode instabilities and dynamic patterns in a colony of self-propelled surfactant particles covering a thin liquid layer*, A. Pototsky, U. Thiele and H. Stark, Europ. Phys. J. E, 39, 51 (2016)
- *Stability of liquid films covered by a carpet of self-propelled surfactant particles*, A. Pototsky, U. Thiele and H. Stark, Phys. Rev. E, 90, 030401(R) (2014)

Models of biofilms



swimmer size $\cdots \sim 1\ \mu\text{m}$

film thickness $\cdots \sim (10\mu\text{m} \ldots 1\ \text{mm})$

swimmer velocity $\cdots \sim 1\mu\text{m/s}$

Applications: biofilms, biocoatings

Model assumptions

Swimmers:

- point-like active Brownian particles
- hydrodynamic interactions neglected
- no alignment of swimming directions

Liquid film:

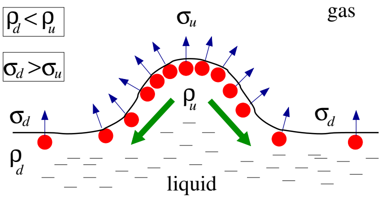
- small Reynolds number flow
- lubrication (long-wave) approximation

particle-liquid interaction

- soluto-Marangoni effect
- particle-induced thin film instability

Particle-induced thin film instability

Sergio Alonso and Alexander Mikhailov, PRE 79, 061906 (2009)

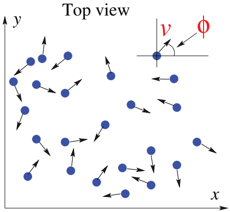


$\rho(x, y) \ldots$ **local particle density at the liquid-gas interface**

$$\text{exess pressure} = \frac{\rho(x, y)\langle v_\perp \rangle}{M} = \alpha \rho(x, y)$$

Modeling bacteria: active Brownian motion

In-plane self propulsion velocity:



$$v\boldsymbol{p} = v(\cos\phi, \sin\phi)$$

Alignment: $\mu(|\, \boldsymbol{r}_i - \boldsymbol{r}_k \,|)$
Rotation frequency: ω_0
Surface fluid velocity at $\boldsymbol{r}_i$: $\boldsymbol{U}_i$

$$\begin{aligned} \dot{\boldsymbol{r}}_i &= v\boldsymbol{p}_i + \boldsymbol{U}_i + \boldsymbol{\xi}_i, \\ \dot{\phi}_i &= \eta_i + \omega_0 + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{U}_i)_z - \sum_{k \neq i} \mu(|\, \boldsymbol{r}_i - \boldsymbol{r}_k \,|) \sin(\phi_i - \phi_k) \end{aligned}$$

with

$$\langle \xi_i(t)\xi_k(t')\rangle = 2Mk_BT\delta_{ik}\delta(t-t'), \quad \langle \eta_i(t)\eta_k(t')\rangle = 2D_r\delta_{ik}\delta(t-t').$$

Smoluchowski equation

Swimmers density:

$$\rho = \rho(x, y, \phi, t)$$

Smoluchowski equation:

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{J}_t + \partial_\phi J_\phi = 0.$$

Translational and rotational currents

$$\boldsymbol{J}_t = v\boldsymbol{p} + \boldsymbol{U}\rho - Mk_B T \boldsymbol{\nabla}\rho$$

$$\begin{aligned} J_\phi &= \left(\omega_0 + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{U})_z\right)\rho - D_r \partial_\phi \rho \\ &- \int\int d\phi' d\boldsymbol{r}' \rho_2(\boldsymbol{r}, \phi, \boldsymbol{r} + \boldsymbol{r}', \phi + \phi')\mu(r', \phi') \end{aligned}$$

Alignment is treated according to Grossmann *et al*, **PRL 258104 (2014)**

Coupling with the thin film equation

Direction-averaged density and soluto-Marangoni effect

$$\langle\rho\rangle(x,y,t) = \int_0^{2\pi} \rho(x,y,\phi,t)\,d\phi, \quad \sigma = \sigma_0 - \Gamma\langle\rho\rangle$$

Thin film equation

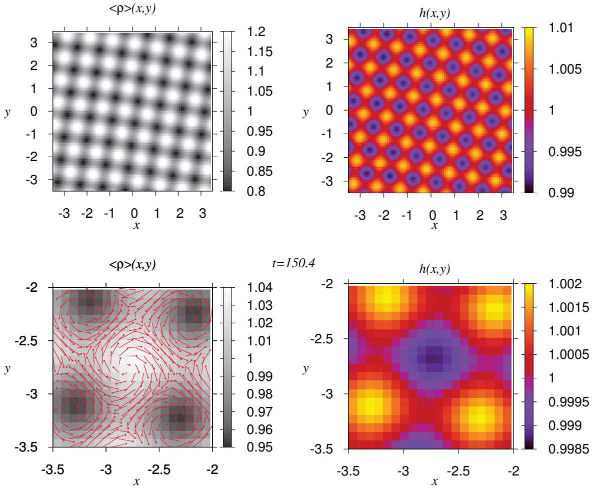
$$\frac{\partial h}{\partial t} + \boldsymbol{\nabla}\cdot\left(\frac{h^3}{3\mu}\boldsymbol{\nabla}\left[\sigma_0\Delta h + \alpha\langle\rho\rangle\right]\right) + \boldsymbol{\nabla}\cdot\left(\frac{h^2}{2\mu}\boldsymbol{\nabla}\sigma\right) = 0$$

Surface fluid velocity

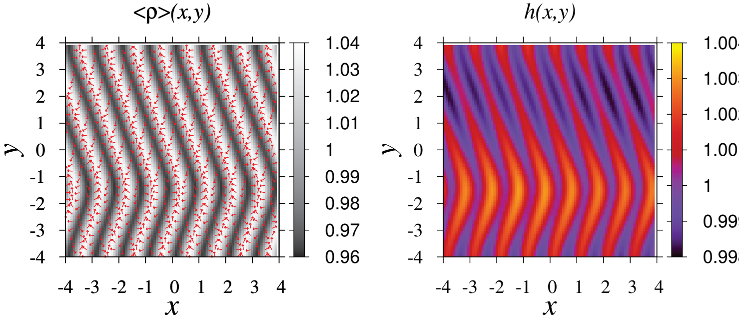
$$\boldsymbol{U} = \frac{h}{\mu}\boldsymbol{\nabla}\sigma + \frac{h^2}{2\mu}\boldsymbol{\nabla}\left(\sigma_0\Delta h + \alpha\langle\rho\rangle\right)$$

Zoo of dynamic density patterns

Square lattice of pulsating vortices



Stripy state



Zoo of dynamic density patterns

Large-scale holes and film rupture